Propane, 2-methyl-2-nitro-

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 135 °C

Global applicability domain: Inside

Local applicability domain index: 8.86e-01

Confidence level: 8.47e-01

Nearest Neighbors from the Training Set

Image not found
Propane, 2-methyl-2-nitro-
Measured: 127
Predicted: 135

Image not found
2-Nitrobutane
Measured: 140
Predicted: 140

Image not found
Propane, 2-methyl-1-nitro-
Measured: 141
Predicted: 140

Image not found
1-Nitrobutane
Measured: 153
Predicted: 144

Image not found
2-Nitropropane
Measured: 120
Predicted: 124